

Special Issue

In Silico Approaches to Unravelling Toxicity Mechanisms in Molecular Drugs

Message from the Guest Editor

This Special Issue will showcase state-of-the-art research focused on data-driven strategies for elucidating drug-induced toxicities and developing predictive models. We welcome submissions addressing various facets of computational toxicology, including the design and application of quantitative structure–activity relationship (QSAR) models, machine learning and artificial intelligence–based algorithms for toxicity prediction, the development and integration of toxicity databases, and in silico analyses aimed at garnering mechanistic insights into toxicity pathways. Studies combining omics data with cheminformatics for holistic toxicity assessments, as well as those identifying novel toxicity biomarkers and incorporating them into predictive frameworks, are particularly encouraged.

Guest Editor

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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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